Ethyl 3-ethoxypropionate 763-69-9 | DTXSID0027309

Model Performance

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Weighted KNN model

5-fold CV (5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.89	0.25	0.88	0.26	0.75	0.38	

Model Results

Predicted value: 4.13 days

Global applicability domain: Outside

Local applicability domain index: 2.31e-01

Confidence level: 8.16e-01

Nearest Neighbors from the Training Set

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2-Methylhexane Measured: 12.5 Predicted: 5.54 Image not found

2-Methylheptane Measured: 12.5 Predicted: 3.99 Image not found

3-Methylhexane Measured: 157 Predicted: 6.83

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2-Methyloctane Measured: 40.7 Predicted: 4.23